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Debye characteristic temperature for liquid metals

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A function similar to the Debye characteristic function has been developed for the liquid metals considering the liquid to have short range order as that of the crystalline state. The specific heats for some liquid metals has been calculated and compared with the experiments. In some cases the results agrees well

1. INTRODUCTION

Debye characteristic temperature is a characteristic function of the crystalline substances which leads to calculation and gaining concept of general physical phenomena. In the case of liquid metals the concept of the Debye characteristic function has not been applied because of the fact that the liquids does not have crystalline order.

Attempts has been made to find the connection between the atomic distribution in liquid and solid metals by Klein & Rupersberg (1967), Rupersberg & Hictor (1975) and others from the similarity of the radial distribution function obtained from X-ray scattering data. The existence of the long range oscillatory potential energy function for the liquid metals have been shown by Johnson *et al* (1963) and Sengupta & Guha (1973). All these data shows the existence of crystalline short range order and partial long range ordor exists in liquid metals.

In the present paper we have attempted to set up a function in case of liquid metals which is similar to that of the Debye characteristic function of solids from the radial distribution function and the X-ray line broadning.

2. METHOD

The radial distribution function $\rho(r)$ for an amorphos solid or a liquid is given by (James 1962)

$$4\pi r^2\rho(r) = 4\pi r^2\rho(0) + \frac{2r}{\pi}\int_0^\infty si(s)e^{-b^2s^2}\sin rsds \qquad \ldots (1)$$

taking into effect of thermal vibration.

where,

$\rho(0)$ = Average density of the molecules in the sample

$s = \frac{4\pi \sin\theta}{\lambda}$ i.e , solid angle subtended by the scattered ray

and λ = The wavelength of the incident ray

$i(s)$ is defined by the relation

$$i(s) = \frac{I(s)}{I(\infty)} - 1$$

where $I(s)$ is the experimental intensity function for the scattered beam, and $I(\alpha)$ = intensity of the scattered beam at $r = \alpha$. $e^{-b^2 s^2}$ is the artificial temperature factor which is account for the thermal agitation of the molecules. As the temperature increases the thermal agitation increases In the liquid state though the thermal agitation is much more than the solids still there is no complete disorderness. Even in the liquids the long range order exists upto 12 to 14Å. This clearly indicate that the concept of Debye characteristic temperature can be extended to the liquid state also

From the radial distribution curve we have the integral breadth 2β which is connected to the amplitude of thermal vibration μ and b^2 as

$$\beta^2 = \frac{\mu^2}{3} + b^2 \qquad \ldots (2)$$

Now we can write,

$$\frac{8\pi^2\mu^2}{3} = \frac{6h^2}{mkT} = f(x) \qquad \ldots (3)$$

where

h = Planck constant
k = Boltzmann const.
T = Temperature in °K
m = mass of the atom

and the function

$$f(x) = \left[\frac{\phi(x)}{x^2} + \frac{1}{4x} \right]$$

where

$$\phi(x) = \frac{1}{x} \int_0^x \frac{\xi d\xi}{e^\xi - 1}$$

and

$$x = \frac{\Theta}{T} \qquad \ldots (4)$$

In the above eq. (4), Θ is a characteristic function similar to the Debye characteric temperature in solids. Expanding and rearranging eq. (1) we have

$$4\pi r^2[\rho(r)-\rho(0)] \quad 2\pi \left[\int si(s) \sin rsds - b^2 \int s^2 i(s) \sin rsds \right] \tag{5}$$

integrating the above equation we get the values of b. Then by using eqs. (3) and (4) the values of $f(x)$ is calculated. From $f(x)$ vs x curve, Θ the characteristic function is find out for different substances

3 Discussions

The result shows that the specific heat calculation made for mercury and sulfer from the function Θ agrees well with the experiment. In case of other liquid metals the results are not so good. This means that the theoretical formulation of the specific heat from this function Θ has to be derived separately and thus a fairly consistant formulation can be made in the case of liquid metals similar to that of solids The theory of the liquid state developed by Hictor *et al* (1967) from the Einstein characteristic temperature also shows that the concept of the diffused solid with the existence of the short range crystalline order can be made. Hictor *et al* (1967) developed the model of the surrounded atoms and considered the Einstein characteristic temperature and vibration of the surrounded atoms. The results obtained for the enthalpy and entropy of a mixture agreed well with the experiment. Thus both Hictor's result and our calculation for C_v from the characteristic function then that the concept of the Debye characteristic function can be extended to that of the liquid metals.

Table 1

Substances	Temp.	C_v in Cal/deg. experimental	C_v in Cal/deg. calculated	Θ
Na	373°K	6·71*	4·25	1007·10
S	353°K	5·21** at 316°K	5·93	105·90
	393°K	—	5·43	534·48
Hg	298°K	5·44† at 293°K	5·11	530·44
Viterious Silica	300°K	—	4·54	726·00

* Klepp (1950)

** Eastman & McGavock 1937

† Bridgeman (1911).

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